

Total ozone determinations from NOAA operational SBUV/2 observations: an update

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Abstract

Total ozone amounts have been derived from observations of the SBUV/2 instruments on NOAA operational satellites since 1985. The data from the NOAA-9 instrument for the period 1985-1997 have been reprocessed using instrument characterizations based on in-orbit operation and comparisons with SSBUV observations. The data from the NOAA-11 satellite for the period 1989-1994 have also been reprocessed using mainly internal spacecraft information. The data from the NOAA-14 satellite for the period 1995-1998 have been reprocessed using complete instrument characterization. The NOAA-11 and NOAA-14 data for 1998-present briefly discussed herein are preliminary. The calibration adjustments used in the reprocessing of NOAA-9, NOAA-11, and NOAA-14 total ozone data are internal with exceptions of those derived from SSBUV analysis and are independent of Dobson and TOMS total ozone measurements. The reprocessed data have been validated with ground-based Dobson spectrophotometer observations, and are compared to other sources of total column ozone amounts. The mean bias between NOAA-9 data and Dobson data is $1.9\% \pm 0.6\%$ over the twelve year record with a trend of about 0.1% per year. The mean bias between NOAA-11 and Dobson data is $0.8\% \pm 0.2\%$ with a near zero trend. The mean bias between NOAA-14 and Dobson data is $1.5\% \pm 0.3\%$; the NOAA-14 calibration and characterization data for the period 1998-present are not yet fully analyzed and have a trend of about 0.2% per year. The methods used in the validations are discussed here as are some reasons for the results. Finally, a recommendation is made for the use of a relatively continuous total ozone data set.

Introduction

Total ozone determinations have been made by the backscattered ultraviolet (buV) technique since the launch of BUUV on Nimbus-4 in 1970. In November 1978, the Solar Backscattered Ultraviolet instrument (SBUV) and the Total Ozone Mapping Spectrometer (TOMS) capable of deriving vertical ozone profiles and total ozone amount were launched on Nimbus-7 by NASA (*Heath et al.*, 1975). A second generation SBUV instrument, SBUV/2, was launched by NOAA on the NOAA-9 operational satellite in 1984 and follow-on NOAA -11, -14 and -16 satellites (*Frederick et al.*; 1986, *Hilsenrath et al.*, 1995). This record covers the period from 1985 to the present. Combining the Nimbus -7 and NOAA data sets gives a potential single data set, SBUV(/2), from 1979 to the present derived from similar instruments.

The SBUV(/2) data set is being used in many areas of atmospheric interest, including ozone trend assessment (see, *e.g.*, *World Meteorological Organization (WMO)*, 1995; *Hollandsworth et al.*, 1995; *Miller et al.*, 1996; *Planet et al.*, 1994 and *Chandra et al.*, 1996) and Ultraviolet Index forecasts (*Long et al.*, 1996). The accuracies attributable to these data and instrumental and other external effects must be clearly known and understood before questions such as trends can be addressed (*e.g.*, *Ahmad et al.*, 1994; *Hilsenrath et al.*, 1995; *McCormack et al.*, 1997). The work presented herein discusses this with respect to instrumental performances and to validation of the satellite-derived total ozone amount by comparisons with ground-based observations.

Instrumental Considerations

The absolute accuracy and long-term repeatability of the ozone data are dependent upon the accuracy to which each SBUV/2 instrument is calibrated and characterized during the instrument's lifetime. These are discussed below for each NOAA instrument separately.

Observations from an instrument are processed daily using the most current instrument characteristics available. In order to create a daily operational ozone product, some aspects of the instrument characterization are simplified by using a constant or extrapolated time dependence.

This allows for a rapid review of the quality of the observational procedures as well as the retrieved ozone products. After a longer period -one or more years- complete instrument characterizations using all available data are generated and the long-term sets of observations are reprocessed to generate a higher-quality data set usable in, for example, trend studies. It is these reprocessed data sets that are the focus of this review.

NOAA-11 Instrument

The previous instrument calibration analysis, used in the first reprocessing (Version 6.0), was based on the first four years of in-flight measurements, from December 1988 through December 1992 (*Hilsenrath et al.*, 1995). The instrument characterization used in the second reprocessing (Version 6.1) was based on the analysis of sensor data taken during December 1988 through April 1995. The NOAA-11 data collection was terminated in April 1995 due to the failure of on-board diffuser and the availability of NOAA-14 data. Due to the bad viewing conditions of NOAA-14 associated with drifting orbit, the NOAA-11 operations were resumed in July 1997 with extrapolated calibration but the ozone product retrieval began only in July 1998 (Huang et al., 2000); the data presented here for the period 1998-present are preliminary.

Because the solar diffuser is the only instrument component not common to the backscattered radiance and solar irradiance measurements from which ozone is derived, accurate knowledge of long-term diffuser reflectivity changes is a key element of the long-term calibration. The SBUV/2 instruments incorporate an on-board calibration system to monitor diffuser reflectivity change (*Frederick et al.*, 1986). *Hilsenrath et al.*, (1995) presented Version 6.0 results. *Steinfeld et al.* (1997) extended this analysis, finding that for the period, 1989-1995, the diffuser degraded approximately linearly in both time and wavelength. The Version 6.1 degradation rate was essentially unchanged from the Version 6.0 characterization. The corrections determined using the onboard calibration data were verified by seven underflights of the NOAA-11 instrument by the Shuttle SBUV (SSBUV) instrument between 1989 and 1994 (*Hilsenrath et al.*, 1995).

The absolute calibration of the NOAA-11 instrument used in the Version 6.0 reprocessing was based on prelaunch calibration information, normalized to the SSBUV absolute calibration. Traditionally, the radiance calibrations of the SBUV/2 and SSBUV instruments require measurements of the bi-directional reflectivity distribution function (BRDF) of a flat-plate laboratory diffuser. These BRDF measurements did not satisfy accuracy and precision requirements, therefore a new calibration technique, using an integrating sphere as the radiance target was employed in the most recent SSBUV calibration (*Janz et al., 1995*). These sphere-based calibrations as well as independent measurements of the flat-plate diffuser's BRDFs revealed a wavelength-independent 5.9% bias in the historical calibrations of the radiance targets. We have therefore adjusted the Version 6.1 radiances downward by 5.9%. This gives rise to an approximate 1.5% adjustment in the derived total ozone value (*Janz et al., 1995*).

The most significant difference between the Version 6.0 and Version 6.1 calibrations for NOAA-11 is in the characterization of the photomultiplier tube (PMT) gain. For operational processing, the Version 6.0 characterization was extrapolated beyond December 1992-1994 on which the Version 6.0 was based. The extrapolation worked well for approximately 8 months, then the actual PMT behavior departed from the predicted behavior, drifting roughly 2.5% near the end of the NOAA-11 data record. The Version 6.1 gain characterization is based on the data record from 1989 to 1994 and therefore accurately tracks the instrument's behavior (*Steinfeld et al., 1997*).

NOAA-9 Instrument

For NOAA-9, the operational ozone product used the Version 5 characterization, which covered the period 1985-1990, as updated with June 1994 calibration information to describe the instrument for that year's Antarctic ozone hole season (*Lienesch et al., 1995*). Unlike the NOAA-11 V6.0 operational processing, the V5 NOAA-9 operational processing did not include a correction for diffuser degradation or any other time-dependent corrections. The V6.1 characterization (*Taylor et al., 2000*) includes complete calibration information and is based on data taken between April 1985 and December 1997. The satellite orbit precessed, and at the end of 1990, it had an equator crossing time around 6:00am (Figure 1). Thus the data for 1990 and 1991 were taken, for the most part, at very high zenith angles and are much less accurate than the

other portions of the data record. As with NOAA-11, the NOAA-9 instrument's V5 absolute calibration was based on the use of flat-plate laboratory diffusers. The V6.1 calibration was transferred to NOAA-9 via SSBUV under-flights and includes the 5.9% adjustment discussed previously.

The NOAA-9 SBUV/2 onboard calibration system failed shortly after launch (*Frederick et al.*, 1986), therefore changes in the diffuser had to be tracked by other means. The D-pair total ozone (derived using radiances measured at 306 and 313 nm channels) in the tropics was used as in-flight calibration standard; D-pair total ozone which is valid only near the equator for solar zenith angles less than 60° is less sensitive to a wavelength dependent calibration drift (Bhartia et al., 1996). The solar zenith angles for the time period between 1989 and 1993 were larger than 60° due to NOAA-9 drifting orbit resulting in invalid D-pair total ozone measurements. Therefore, the calibration for this time period was interpolated between the earlier period (1985-1989) and later period (1993-1997). The revised calibration for the PMT non-linearity in gain range 3 was obtained by processing the SBUV/2 data through a specially developed ozone algorithm based on the TOMS Version 7 processing (McPeters, 1994); this algorithm generates channel residues which are differences between measured and calculated radiances. The differences in channel residues for measurements under different viewing conditions (high reflectivity vs low reflectivity) were used to determine the non-linearity in PMT gain range 3. Additional errors in the PMT characterization due to hysteresis effect when the satellite comes out of the earth's dark side have also been corrected (DeLand et al., 2000).

NOAA-14 Instrument

The NOAA-14 instrument was launched in January 1995. Before the instrument could be well characterized after launch and the data record reprocessed, it experienced problems with cloud cover radiometer and the grating drive. The instrument suffered the failure of its cloud cover radiometer which is used to monitor scene reflectivity changes. The monochromator wavelength selection was changed by dropping a profiling wavelength, adding another reflectivity

measurement, and changing the order of measurement to provide scene reflectivity monitoring (DeLand et al., 1998). The grating drive started to experience an anomalous operating condition which caused sampling slightly away from planned wavelength positions. This resulted in changes in the procedure to account for wavelength errors. Even after the correction is applied, some additional noise is present. The characterization of PMT gain changed by about 7% in the first three years of operation affecting the operational product. But this was fully treated in the V6 reprocessed product for 1995-1998 discussed here. The calibration for the time period 1995-1998 was extrapolated beyond 1998 to continue the measurements and retrieval of the ozone products and to apply a degree of validation.

Validation Data

The primary source of validation data is the global network of Dobson spectrophotometers sponsored by the World Meteorological Organization (WMO). Dobson instruments are themselves sources of long-term data sets (*Komhyr et al., 1997; Bojkov and Fioletov, 1995*) as well as sources of data for validating satellite data records. A subset of the global network that is either operated directly or cooperatively by the NOAA Climate Monitoring and Diagnostic Laboratory (CMDL) (<http://www.cmdl.noaa.gov/owv>) is a major source of the ground data used in our validation of the SBUV/2 data discussed herein.

The Dobson stations providing data for our purpose are shown in Table 1 where asterisks denote the CMDL sub-set containing ten stations. Data from all Dobson stations are obtained from the World Ozone and Ultraviolet Radiation Data Center (WOUDC) in Toronto, Canada (<http://www.msc-smc.ec.gc.ca/woudc>). The Dobson-derived total ozone data records currently archived at the WOUDC are the most accurate to-date. The CMDL data have recently been re-evaluated and have been used to infer trends at their respective locations (*Komhyr et al., 1997*).

The CMDL Dobson monthly data products are sent to the WOUDC with a lag of about 3 to 4 months after observation. The WOUDC maintains an archive of data from more than 100 stations globally. Comparison match-ups of satellite and ground-based Dobson observations are routinely

performed for operational and reprocessed satellite data for validation purposes. We have selected twenty-one stations for our match-up procedure based on report reliability, consistency, and length of record. For both Dobson data sources, CMDL (a sub-set of ten stations) and WOUDC, total ozone amount in Dobson Units (DU) and time of observation are reported on a daily basis. Satellite data are screened for good observations (*e.g.*, measurements made at solar zenith angles greater than 80° are not used) and match-ups are performed if a satellite retrieval occurs within a 3-degree arc circle of a Dobson station. If the difference in time of each observation is less than 12 hours, a match-up is made. If more than one satellite retrieval occurs within the coincidence circle, a simple average value is used in the comparison. Each station must have at least 5 daily matches per month in order to produce a monthly mean difference for that station. Statistics are generated on monthly mean difference for that station. Means, standard deviations and standard errors of the differences are produced monthly for each station. The mean difference (in %) is the most commonly used parameter here and is calculated as

$$100 [\text{Satellite ozone} - \text{Dobson ozone}] / \text{Dobson ozone}, \%$$

For each month, these mean differences at each station are then summed. An average mean monthly difference is then available for the ensemble of all stations used in the analysis. The average mean monthly difference is not used if the ensemble is less than six; the only exception is for NOAA-11 comparisons for the time period 1998-present where we changed the criteria to a minimum of four stations because some CMDL stations have missing Dobson data.

Data Comparisons

Comparisons of the NOAA-9,-11 and-14 total ozone amounts are discussed here relative to the ground-based CMDL Dobson data records and total ozone amounts derived from observations of the NASA Total Ozone Mapping Spectrometer (TOMS) on the NASA Nimbus-7 research satellite launched in 1978 (*McPeters et al.*,1996a;*Fleig et al.*, 1990). The SBUV/2 ozone retrievals were

computed with the Version 6.1 SBUV algorithm while the TOMS data were computed with the Version 7 TOMS algorithm (McPeters et al., 1996).

Dobson total ozone amount

A comparison of the differences between the NOAA-11 SBUV/2 total ozone amount and those from the WOUDC (solid line) and the CMDL (dashed line) data sets are shown in Figure 2. Very good agreement is demonstrated with trends in the differences between NOAA-11 and the WOUDC data set of -0.1 %/yr and the CMDL data set of 0.0 %/yr over the period of the NOAA-11 observations. Figure 3 presents the differences between the total ozone amounts derived from the NOAA-9, -11 and -14 observations and those from the CMDL stations Dobson observations (We use the CMDL data set to be consistent with its use in the earlier stages of data validation. These data were obtained from CMDL and are consistent with those archived at WOUDC) Also included in Figure 3 are comparisons of the NASA Nimbus-7 SBUV. For NOAA-11, we note that there is a bias of 0.8 % in the differences with essentially no time dependence during 1989-1994. For NOAA-9, there are two distinct comparison periods. The first covers the time from launch until the end of 1990 when the space craft in the ascending node approaches the terminator and the solar zenith angles go beyond 85 degrees where the ozone retrieval algorithm is no longer valid. Starting early 1991, the spacecraft is in the descending node. The data for NOAA-9 for the 10-month period around 1991 are excluded from the analysis due to the fact that all observations were made near the terminator and the large solar zenith angles are not accommodated by the retrieval algorithm. There is a mean bias of about 2.0% during the entire time period with a not yet understood small upward drift toward the end of the record.

The total ozone zonal averages near the equator retrieved from reprocessed NOAA-14 observations are about 1% to 2% lower than those of NOAA-9 when there was overlapping coverage by the two satellites. Similar differences exist between direct comparisons of NOAA-9 and NOAA-11. These differences agree with SBUV/2 and Dobson data comparisons shown in Figure 2.

TOMS total ozone amount

Total ozone amounts derived from the NOAA observations have been compared with those derived from the Nimbus-7 TOMS observations starting in 1985. We note that the TOMS data presented here were retrieved with the NASA Version 7 algorithm while the SBUV/2 data were retrieved with the Version 6 algorithm. TOMS data were previously compared with Dobson data (*McPeters and Labow, 1996b*) and it is instructive to look at SBUV/2 -and TOMS- Dobson comparison results even though the Dobson data sets for each comparison were different. Comparisons were made of zonal averages in that the footprints of the SBUV/2 and TOMS are very different and TOMS is a scanning instrument while SBUV/2 is a nadir-only instrument. Figure 4 presents the monthly differences, $[\text{NOAA-11 total ozone} - \text{TOMS total ozone}] / \text{TOMS total ozone}, \%$, for three latitude regions of the globe. Figure 5 presents the same type of comparisons but with NOAA-9 data. The NOAA-11 comparison in Figure 4 shows agreement to approximately $\pm 0.5\%$ over the 4-year overlap period. The sharp difference in 1992 is due to measurements made at large solar zenith angles by the SBUV/2 in the southern hemisphere winter. The NOAA-9 comparison, however, shows a flat agreement over the first two years. After that, the difference shows a small time-dependence. This is consistent with the NOAA-9 comparison with Dobson data shown in Figure 3. The reason for this variation is not known.

Discussion

The SBUV/2 instruments use combinations of measurements at four wavelengths (corrected for scene reflectivity changes by using the photometer) to obtain the best estimates of the total amount. Estimates are obtained from three pairs of these wavelengths, viz, A-pair uses the 313 and 331 nm channels, B-pair uses the 318 and 331 nm channels and C-pair uses the 331 and 340nm channels. In general, the A-pairs are given the most weight for low solar zenith angle retrievals, the C-pair for high angles and the B-pair for intermediate angles. Computing differences between two pairs total ozone estimates where both should produce good results can serve as an internal monitor of calibration consistency (*Herman et al., 1991*). Figure 6 shows the

time series of differences between the A-pair and B-pair total ozone estimates from NOAA-9 and NOAA-11 for the 25 degree latitude zone around the equator. The offsets between total ozone estimates from A-pair and B-pair are due to wavelength dependent calibration error (between 313 and 318 nm), differences in A-pair and B-pair sensitivities to ozone profile shape and solar zenith angle, and assumptions of wavelength independent effective reflectivity. Though there are small drifts (0.1% to 0.2% per year) over shorter time periods, there is no significant trend in the data during the 12-year data record; this is consistent with the good agreement observed with the Dobson measurements.

Conclusion

The NOAA-9, -11, and -14 total ozone data were reprocessed with internal calibration adjustments with exceptions of those derived from SSBUV analysis and are independent of Dobson and TOMS total ozone measurements. Comparisons of the total ozone data from the NOAA SBUV/2 instruments on the NOAA-9, -11 and -14 satellites show an overall general agreement with that from Dobson ground-based and Nimbus-7 TOMS data over the period from late 1984 to present. The NOAA-9 comparisons with Dobson data show a bias of 1.9% with a trend in the bias of about 0.1% per year; this trend is significantly less than the trends observed in total ozone for mid latitudes (WMO, 1999). The NOAA-11 comparisons with Dobson data show a bias of 0.8% with near zero trend in the bias for the period 1989-1994 during which the instrument was well characterized. The NOAA-11 and NOAA-14 data for 1998-present are yet to be fully characterized. Though there are trends of about 0.1% to 0.2% per year in comparisons of SBUV data with either Dobson or TOMS data on shorter time periods, the overall trend in the difference between SBUV and Dobson data over the 20-year data record is only 0.6% per decade. Satellite to satellite differences of up to 2% in total ozone measurements are observed for Nimbus-7, NOAA-9, NOAA-11, and NOAA-14 during their overlaps; differences in absolute instrument calibration on these satellites contribute to this bias. A 20-year continuous SBUV total ozone data set can be created by adjusting satellite to satellite biases using the overlap data screened for good viewing conditions (good solar zenith angles) and contamination from volcanic aerosols. The data

sets are available to scientific community by anonymous ftp at [orbit35i.nesdis.noaa.gov/pub/crad2](ftp://orbit35i.nesdis.noaa.gov/pub/crad2) for total ozone trend assessments.

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Table 1: Locations of Dobson Sites

52.5	Post dam, Germany
52.3	Belsk, Poland
50.8	Uccle, Belgium
50.2	Hradec Kralove, Czech Republic
46.8	*Caribou, USA
46.7	Arosa, Switzerland
46.7	* Bismark, USA
44.5	Haute Provence, France
43.7	Toronto, Canada
40.0	*Boulder, USA
39.9	Xianghe, China
37.8	*Wallops Island, USA
36.7	*Fresno, USA
36.2	*Nashville, USA
36.0	Tateno, Japan
30.0	Cairo, Egypt
25.3	Varanasi, India
19.5	*Mauna Loa, USA
18.5	Poona, India
1.3	Singapore, Singapore
-12.0	*Huancayo, Peru
-14.0	*Samoa, USA
-31.8	*Perth, Australia

Figure 1: The time series of the local equator crossing time (hours) for NOAA-9, NOAA-11, and NOAA-14.

Figure 2: Differences between NOAA-11 total ozone amount and that from the WOUDC (solid line) and CMDL (dashed line) in percent over life of NOAA-11 observations.

Figure 3: Differences between NOAA-9, -11, and -14 total ozone amounts and that from CMDL Dobson observations. The red circles are Nimbus-7 SBUV data, the green inverted triangles are NOAA-9 data, the red asterisks are NOAA-11 data, and the black squares are NOAA-14 data.

Figure 4: Differences between NOAA-11 SBUV/2 total ozone amount and that from Nimbus-7 TOMS for 30N-50N (dotted line), 30S-50S (dashed line), 25S-25N (solid line).

Figure 5: Same as Figure 4 but for NOAA-9 data.

Figure 6: A-pair, B-pair total ozone amount differences for 25N-25S zone and solar zenith angles less than 70 degrees for NOAA-9 and NOAA-11.

Acronyms

BRDF	Bidirectional Reflectivity Distribution Function
CMDL	Climate Monitoring Diagnostic Laboratory
DU	Dobson Units
NOAA	National Oceanic and Atmospheric Administration
PMT	Photomultiplier Tube
SBUV	Solar Backscatter Ultraviolet
SSBUV	Shuttle Solar Backscatter Ultraviolet
TOMS	Total Ozone Mapping Spectrometer
WMO	World Meteorological Organization
WOUDC	World Ozone Ultraviolet Data Center

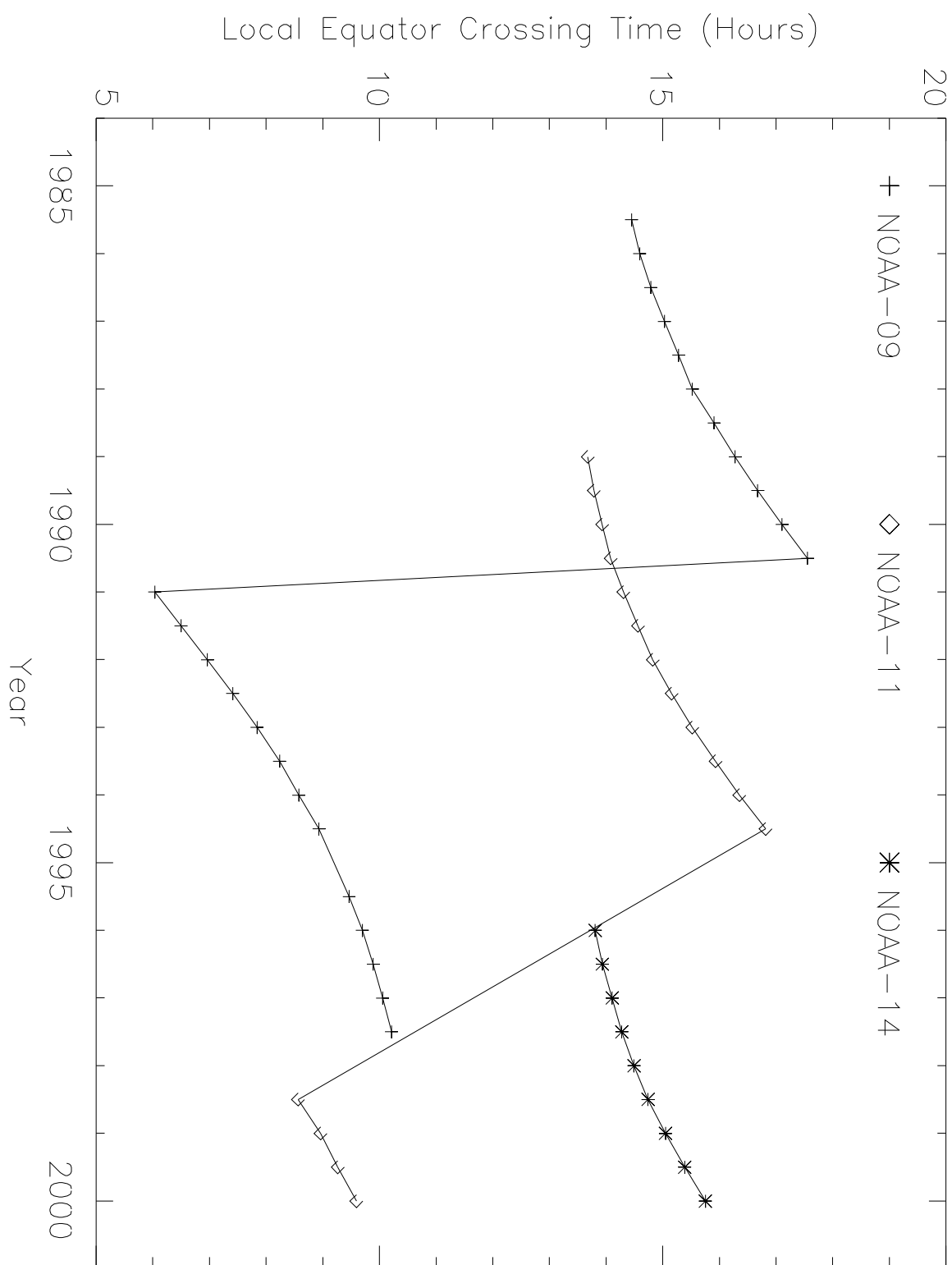


Fig.2:

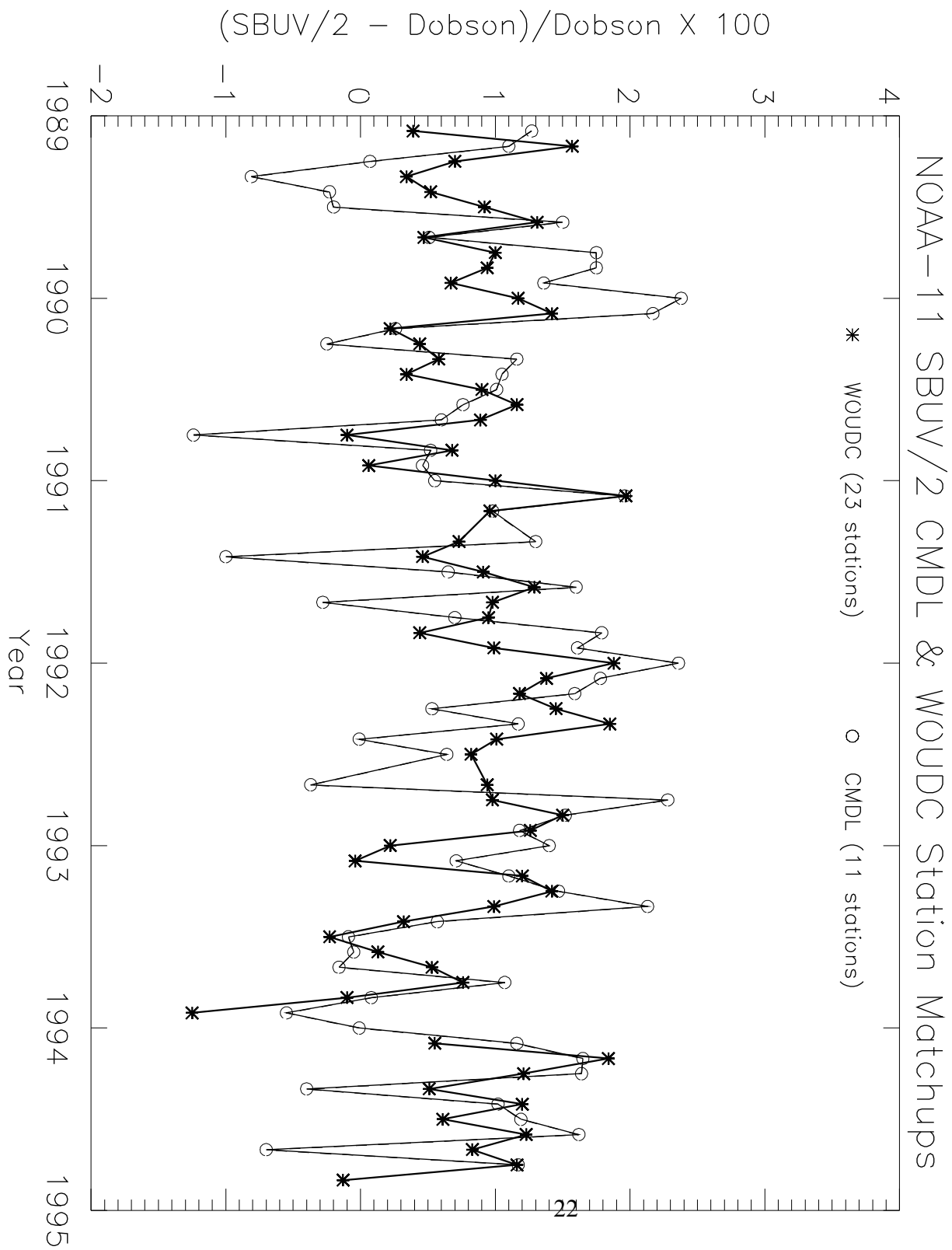


Fig.3:

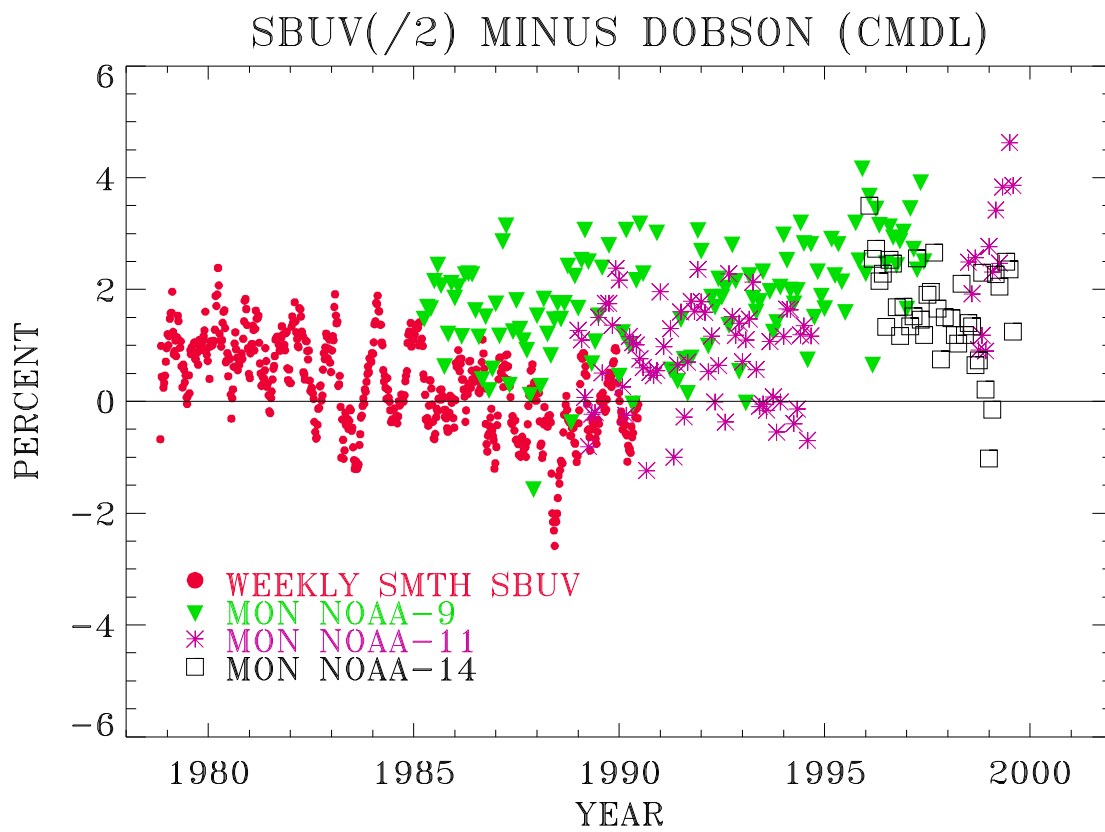


Fig.4:

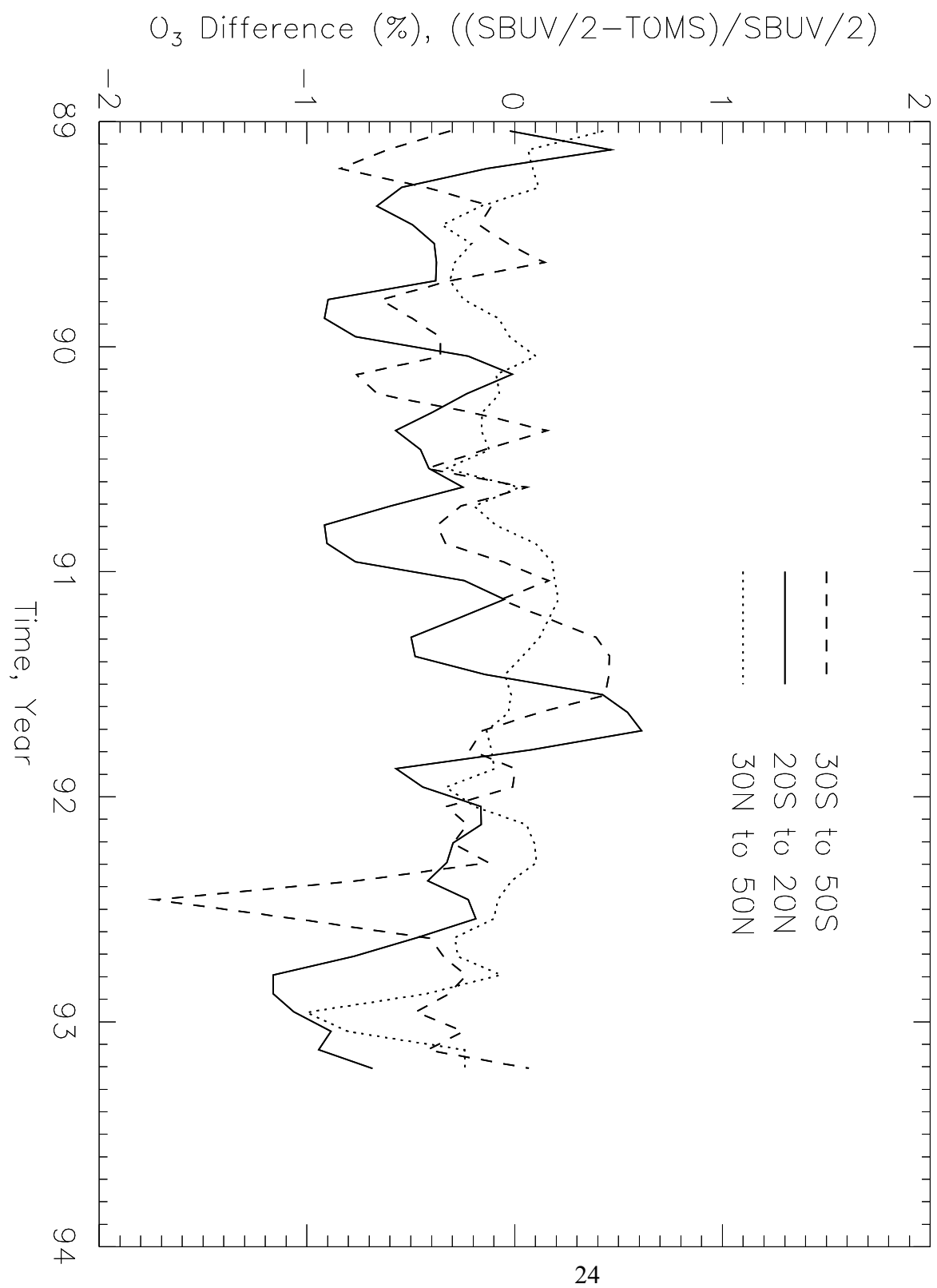


Fig.5:

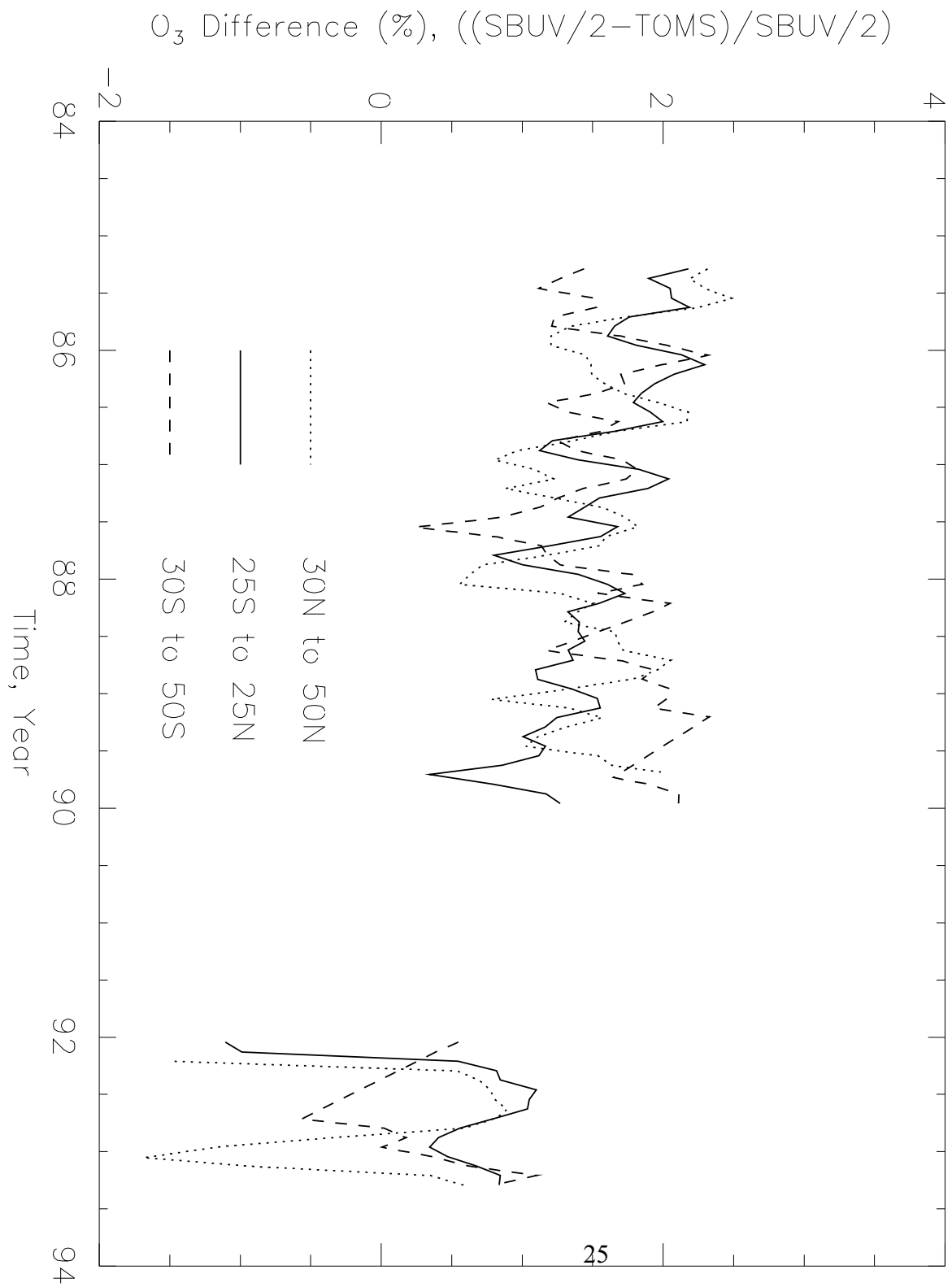


Fig.6:

